# The Wiener Polarity Index of Graph Products *

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**Abstract**

The Wiener polarity index of a graph $G$, denoted by $W_p(G)$, is the number of unordered pairs of vertices $u$, $v$ such that the distance between $u$ and $v$ is three, which was introduced by Harold Wiener in 1947. The Wiener polarity index is used to demonstrate quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons. In this paper, we study the Wiener polarity index on the Cartesian, direct, strong and lexicographic product of two non-trivial connected graphs.

**Keywords**: Wiener polarity index, graphs, graph product

# 1 Introduction

Let $G = (V, E)$ be a connected simple graph. The distance between two vertices $u$ and $v$ in $G$, denoted by $d_G(u, v)$, is the length of a shortest path between $u$ and $v$ in $G$. Let $N_G(v)$ be the neighborhood of $v$, and $d_G(v) = |N_G(v)|$ denote the degree of vertex $v$. For notations and terminology not given here, see e.g. [2] and [19]. The Wiener polarity index of a graph $G = (V, E)$, denoted by $W_p(G)$, is the number of unordered pairs of vertices $\{u, v\}$ of $G$ such that $d_G(u, v) = 3$, i.e.,

$$W_p(G) := |\{\{u, v\}|d(u, v) = 3, u, v \in V(G)\}|.$$

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The name "Wiener polarity index" is introduced by Harold Wiener [18] in 1947. Wiener himself conceived the index only for acyclic molecules and defined it in a slightly different - yet equivalent - manner. In the same paper, Wiener also introduced another index for acyclic molecules, called *Wiener index* or *Wiener distance index* and defined by $W(G) := \sum_{\{u,v\}\subseteq V} d_G(u,v)$. The Wiener index $W(G)$ is popular in both chemical and mathematical literatures. For more results on Wiener index, we refer to the survey paper [8] written by Dobrynin et al.

The Wiener polarity index is used to demonstrate quantitative structure-property relationships in a series of acyclic and cycle-containing hydrocarbons by Lukovits and Linert [15]. Hosoya in [10] found a physical-chemical interpretation of $W_p(G)$. Du et al. [9] described a linear time algorithm APT for computing the Wiener polarity index of trees, and characterized the trees maximizing the Wiener polarity index among all trees of given order. The extremal Wiener polarity index of (chemical) trees with given different parameters (e.g. order, diameter, maximum degree, the number of pendants, etc.) were studied, see [4, 5, 7, 12, 13]. Moreover, the unicyclic graphs minimizing (resp. maximizing) the Wiener polarity index among all unicyclic graphs of order $n$ were given in [11]. Recently, Ma et al. study the extremal Wiener polarity index of unicyclic graphs with a given diameter [17]. Furthermore, the maximum Wiener polarity index of bicyclic graphs is also determined [16]. There are also extremal results on some other graphs, such as fullerenes, hexagonal systems and cactus graph classes, we refer to [1, 3, 6]. In [14], Ilić and Ilić defined the generalized Wiener polarity index $W_k(G)$ as the number of unordered pairs of vertices $\{u,v\}$ of $G$ such that the shortest distance $d(u,v)$ between $u$ and $v$ is $k$ (this is actually the $k$-th coefficient in the Wiener polynomial).

Let $G$ be a graph with $\omega$ components $G_1, \ldots, G_\omega$. Obviously, $W_p(G) = \sum_{i=1}^{\omega} W_p(G_i)$. Thus, to calculate the Wiener polarity index for general graphs, it is sufficient to study how to calculate the index for connected graphs.

For a given connected graph $G$, we define $W_2(G) := |\{\{u,v\} \mid d(u,v) = 2, u,v \in V(G)\}|$, which is the number of unordered pairs of vertices $\{u,v\}$ of $G$ such that $d_G(u,v) = 2$. Actually, for a given graph $G$, we can compute the exact value of $W_2(G)$ in a polynomial time.

In this paper, we study the Wiener polarity index on the Cartesian, direct, strong and lexicographic product of two non-trivial connected graphs.

# 2 The Cartesian Product

In this section, we firstly introduce the Cartesian product of two connected graphs and derive some of its basic properties, and then we are concerned with the Wiener polarity index of the Cartesian product of two non-trivial connected graphs.

The *Cartesian product* of two graphs $G$ and $H$, denoted by $G\Box H$, is defined on the Cartesian product $V(G) \times V(H)$ of the vertex sets of $G$ and $H$. The edge set $E(G\Box H)$ is the set of all pairs $((u,x),\ (v,y))$ of vertices for which either $u = v$ and $xy \in E(H)$ or $uv \in E(G)$ and $x = y$, where $u,v \in V(G)$ and $x, y \in V(H)$. Namely,

$$V(G\Box H) = V(G) \times V(H),$$

$$E(G\Box H) = \{((u,x),\ (v,y)) \mid u = v, xy \in E(H),\ or\ uv \in E(G), x = y\}.$$

The mappings $p_1 : (u,x) \longrightarrow u$ and $p_2 : (u,x) \longrightarrow x$ from $V(G\Box H)$ into $V(G)$ and $V(H)$, respectively, are weak homomorphisms from $G\Box H$ onto $G$ and $H$, respectively. We call them *projections*. Sometimes, we also write $p_G$ and $p_H$ instead of $p_1$ and $p_2$. For a set $S$ of vertices of $G\Box H$, we define $p_i(S) = \{p_i(v) \mid v \in S\}$, where $i \in \{1,2\}$.

For $a = (u,x) \in V(G\Box H)$ ($u \in V(G)$ and $x \in V(H)$), we define $p_1(a) = u$, $p_2(a) = x$. As we noted, $p_i$ ($i = 1,2$) is a weak homomorphism. If we restrict $p_i$ to the subgraph induced by all vertices that differ from a given vertex $b = (v,y) \in G\Box H$ only in $u \in V(G)$ (or $x \in V(H)$), it becomes an isomorphism because

$$< \{u \in V(G) \mid p_2(a) = x\} > \ (or < \{x \in V(H) \mid p_1(a) = u\} >)$$

is isomorphic to $G$ (or $H$). This subgraph is called the *G-layer* (or the *H-layer*).

Now we give some basic properties about the Cartesian product.

**Proposition 2.1** ([19]). The Cartesian product of two graphs $G$ and $H$ is connected if and only if both $G$ and $H$ are connected.

**Lemma 2.1** ([19]). *Let $(u,x)$ and $(v,y)$ be two arbitrary vertices of the Cartesian product $G\Box H$. Then $d_{G\Box H}((u,x),(v,y)) = d_G(u,v) + d_H(x,y)$. Moreover, if $Q$ is a shortest path between $(u,x)$ and $(v,y)$, then $p_1(Q)$ is a shortest path in $G$ from $u$ to $v$ and $p_2(Q)$ is a shortest path in $H$ from $x$ to $y$.*

From Proposition 2.1 and Lemma 2.1, we can get the following theorem.

**Theorem 2.1.** *Let $G$ and $H$ be two non-trivial connected graphs, then*

$$W_p(G\Box H) = W_p(G)V(H) + W_p(H)V(G) + 2W_2(G)m(H) + 2W_2(H)m(G),$$

*where $m(G)$ and $m(H)$ are the number of edges of $G$ and $H$, respectively.*

*Proof.* Since $G$ and $H$ are both non-trivial connected graphs, $G\Box H$ is connected by Proposition 2.1. Let $u,v \in V(G)$, $x,y \in V(H)$ and $(u,x)$, $(v,y) \in V(G\Box H)$. Suppose $a = (u,x)$ and $b = (v,y)$. By Lemma 2.1, we have $d_{G\Box H}(a,b) = d_G(u,v) + d_H(x,y)$. Thus, $d_{G\Box H}(a,b) = 3$ if and only if $d_G(u,v) = 3$ and $d_H(x,y) = 0$, or $d_G(u,v) = 2$ and $d_H(x,y) = 1$, or $d_G(u,v) = 1$ and $d_H(x,y) = 2$, or $d_G(u,v) = 0$ and $d_H(x,y) = 3$. We will consider the following four cases and denote by $W_p^i$ the values of the Wiener polarity index in each case, respectively, $i = 1,2,3,4$.

**Case 1.** $d_G(u,v) = 3$ and $d_H(x,y) = 0$.

Since the mappings $p_1 : (u,x) \longrightarrow u$ and $p_2 : (u,x) \longrightarrow x$ from $V(G\Box H)$ into $V(G)$ and $V(H)$, respectively, are weak homomorphisms from $G\Box H$ onto $G$ and $H$, respectively, we have $W_p^1(G\Box H) = W_p(G)V(H)$.

**Case 2.** $d_G(u,v) = 2$ and $d_H(x,y) = 1$.

Under the condition that $d_G(u,v) = 2$ and $d_H(x,y) = 1$, we know $d_{G\Box H}(a,b) = 3$ if and only if there exists a $u-v$ path $P$ of length two in $G$ and vertices $x$, $y$ are adjacent in $H$. By the mappings $p_1$ and $p_2$, we can get

$$W_p^2(G\Box H) = 2W_2(G)\frac{\sum_{x\in V(H)} d_H(x)}{2} = 2W_2(G)m(H).$$

**Case 3.** $d_G(u,v) = 1$ and $d_H(x,y) = 2$.

Similar to Case 2, we can get

$$W_p^3(G\Box H) = 2W_2(H)\frac{\sum_{u\in V(G)} d_G(u)}{2} = 2W_2(H)m(G).$$

**Case 4.** $d_G(u,v) = 0$ and $d_H(x,y) = 3$.

Similar to Case 1, we have $W_p^4(G\Box H) = W_p(H)V(G)$.

Combining the above four cases, we have

$$W_p(G\Box H) = W_p(G)V(H) + W_p(H)V(G) + 2W_2(G)m(H) + 2W_2(H)m(G).$$

The proof is then complete. □

# 3 The Strong Product

In this section, we first introduce the strong product and then discuss the Wiener polarity index of the strong product of two non-trivial connected graphs.

The *strong product* $G\boxtimes H$ of $G$ and $H$ is defined on the Cartesian product of the vertex sets of $G$ and $H$. Two distinct vertices $(u,x)$ and $(v,y)$ of $G\boxtimes H$ are adjacent with respect to the strong product if

$$u = v \textit{ and } xy \in E(H), \textit{ or } uv \in E(G) \textit{ and } x = y, \textit{ or } uv \in E(G) \textit{ and } xy \in E(H).$$

Now we give some basic properties about the strong product.

**Proposition 3.1** ([19]). The strong product of two graphs $G$ and $H$ is connected if and only if both $G$ and $H$ are connected.

**Lemma 3.1** ([19]). *Let $G\boxtimes H$ be the strong product of connected graphs $G$ and $H$. Then $d_{G\boxtimes H}((u,x),(v,y)) = max\{d_G(u,v), d_H(x,y)\}$, where $(u,x),(v,y) \in V(G\boxtimes H)$, $u,v \in V(G)$ and $x,y \in V(H)$.*

From the above properties, it is not difficult to get the following theorem.

**Theorem 3.1.** *Let $G$ and $H$ be two non-trivial connected graphs, then*

$$\begin{aligned} W_p(G\boxtimes H) =& W_p(G)[2W_p(H) + 2W_2(H) + 2m(H) + n(H)] \\ &+ W_p(H)[2W_2(G) + 2m(G) + n(G)], \end{aligned}$$

*where $m(G)$ and $m(H)$ are the number of edges of $G$ and $H$, respectively, and $n(G)$ and $n(H)$ are the number of vertices of $G$ and $H$, respectively.*

*Proof.* Since $G$ and $H$ are both non-trivial connected graphs, $G \boxtimes H$ is connected by Proposition 3.1. Let $u, v \in V(G)$, $x, y \in V(H)$ and $a = (u, x)$, $b = (v, y) \in V(G \boxtimes H)$. By Lemma 3.1, we have $d_{G\boxtimes H}(a, b) = max\{d_G(u, v),\ d_H(x, y)\}$. Thus, $d_{G\boxtimes H}(a, b) = 3$ if and only if $d_G(u, v) = 3$ and $d_H(x, y) \leq 3$, or $d_H(x, y) = 3$ and $d_G(u, v) \leq 3$. We will give the proof of the theorem by the following two cases and denote by $W_p^i$ the values of the Wiener polarity index in each case, respectively, $i = 1, 2$.

**Case 1.** $d_G(u, v) = 3$ and $d_H(x, y) \leq 3$.

If $d_G(u, v) = 3$ and $d_H(x, y) = 3$, then the value of the Wiener polarity index is $2W_p(G)W_p(H)$. If $d_G(u, v) = 3$ and $d_H(x, y) = 2$, then the value of the Wiener polarity index is $2W_p(G)W_2(H)$. If $d_G(u, v) = 3$ and $d_H(x, y) = 1$, then the value of the Wiener polarity index is $2W_2(G)\frac{\sum_{x\in V(H)} d_H(x)}{2} = 2W_2(G)m(H)$. If $d_G(u, v) = 3$ and $d_H(x, y) = 0$, then the value of the Wiener polarity index is $W_p(G)n(H)$. Therefore,

$$W_p^1(G \boxtimes H) = W_p(G)[2W_p(H) + 2W_2(H) + 2m(H) + n(H)].$$

**Case 2.** $d_H(x, y) = 3$ and $d_G(u, v) \leq 3$.

Similar to Case 1, we can get

$$W_p^2(G \boxtimes H) = W_p(H)[2W_p(G) + 2W_2(G) + 2m(G) + n(G)].$$

By combining the two cases and removing the duplicate part, we have

$$\begin{aligned} W_p(G \boxtimes H) =& W_p^1(G \boxtimes H) + W_p^2(G \boxtimes H) - 2W_p(G)W_p(H) \\ =& W_p(G)[2W_p(H) + 2W_2(H) + 2m(H) + n(H)] \\ &+ W_p(H)[2W_2(G) + 2m(G) + n(G)]. \end{aligned}$$

The proof is complete. □

# 4 The Direct Product

In this section, we introduce the direct product and then we are concerned with the Wiener polarity index of the direct product of two non-trivial connected graphs.

Again, the vertex set of the *direct product* $G \times H$ ($G$ and $H$ are called the factors of $G \times H$) of two graphs is $V(G) \times V(H)$. Two vertices $(u,x), (v,y)$ are adjacent if both $uv \in E(G)$ and $xy \in E(H)$. Note that $E(G \boxtimes H) = E(G \Box H) \cup E(G \times H)$.

The projections $p_i$ of $G \times H$ into $G$ and $H$ are homomorphisms, not just weak homomorphisms as in other respects. For example, in the case of simple graphs, the $G$-layer and $H$-layer which we define as for the Cartesian product, are totally disconnected graphs on $G$ and $H$ vertices.

The connectivity properties of the direct product are also much richer than those of the other two products previously introduced. Although all factors of a connected direct product must be connected, as one can see by projection into the factors, the converse is not true.

**Proposition 4.1** ([19]). Let $G$ and $H$ be graphs with at least one edge. Then $G \times H$ is connected if and only if both $G$ and $H$ are connected and at least one of them is non-bipartite.

**Lemma 4.1** ([19]). *Let $(u,x)$, $(v,y)$ be vertices of $G \times H$ and $P$ be a walk in $G$ connecting $u$ with $v$. Furthermore, let $Q$ be a walk from $x$ to $y$ in $H$, and suppose that $|E(P)| + |E(Q)|$ is even. Then there exists a path in $G \times H$ from $(u,x)$ to $(v,y)$.*

**Theorem 4.1.** *Let $G$ and $H$ be two non-trivial connected graphs and at least one of them is non-bipartite, then*

$$W_p(G \times H) = 2W_p(G)W_p(H) + 2W_p(H)m(G) + 2W_p(G)m(H),$$

*where $m(G)$ and $m(H)$ are the number of edges of $G$ and $H$, respectively.*

*Proof.* Since $G$ and $H$ are both non-trivial connected graphs and at least one of them is non-bipartite, $G \times H$ is connected by Proposition 4.1. Let $u, v \in V(G)$, $x, y \in V(H)$ and $a = (u,x)$, $b = (v,y) \in V(G \times H)$. By Lemma 4.1, there exists a path in $G \times H$ from $(u,x)$ to $(v,y)$ on condition that there is a walk $P$ in $G$ connecting $u$ with $v$ and a walk $Q$ in $H$ connecting $x$ and $y$ such that $|E(P)| + |E(Q)|$ is even. Therefore, $d_{G\times H}(a,b) = 3$ if and only if $|E(P)| = 1$ and $|E(Q)| = 3$, or $|E(P)| = 3$ and $|E(Q)| = 1$, or $|E(P)| = 3$ and $|E(Q)| = 3$ (i.e., $d_G(u,v) = 1$ and $d_H(x,y) = 3$, or $d_G(u,v) = 3$ and $d_H(x,y) = 1$, or $d_G(u,v) = 3$ and $d_H(x,y) = 3$). We continue the proof of our theorem by the following three cases and denote by $W_p^i$ the values of the Wiener polarity index in each case, respectively, $i = 1, 2, 3$.

respectively.

**Case 1.** $d_G(u,v) = 1$ and $d_H(x,y) = 3$.

Since $d_H(x,y) = 3$ and $u$ is adjacent to $v$ in $H$, we get

$$W_p^1(G \times H) = 2W_p(H)\frac{\sum_{u \in V(G)} d_G(u)}{2} = 2W_p(H)m(G).$$

**Case 2.** $d_G(u,v) = 3$ and $d_H(x,y) = 1$.

Since $d_G(u,v) = 3$ and $x$ is adjacent to $y$ in $H$, we get

$$W_p^2(G \times H) = 2W_p(G)\frac{\sum_{x \in V(H)} d_H(x)}{2} = 2W_p(G)m(H).$$

**Case 3.** $d_G(u,v) = 3$ and $d_H(x,y) = 3$.

In this case, we have $W_p^3(G \times H) = 2W_p(G)W_p(H)$.

By combining the above three cases above, we have

$$W_p(G \times H) = 2W_p(G)W_p(H) + 2W_p(H)m(G) + 2W_p(G)m(H).$$

The proof is thus complete. □

# 5 The Lexicographic Product

This section is concerned with the lexicographic product with respect to the Wiener polarity index.

The *lexicographic product* $G \circ H$ of two graphs $G$ and $H$ is defined on $V(G \circ H) = V(G) \times V(H)$, two vertices $(u,x)$, $(v,y)$ of $G \circ H$ being adjacent whenever $uv \in E(G)$, or $u = v$ and $xy \in E(H)$. Note that the lexicographic product $G \circ H$ can be obtained from $G$ by substituting a copy $H_v$ of $H$ for every vertex $v$ of $G$ and by joining all vertices of $H_v$ with all vertices of $H_u$ if $uv \in E(G)$.

**Proposition 5.1** ([19]). Let $G$ and $H$ be two nontrivial graphs, namely, graphs with at least two vertices. Then $G \circ H$ is connected if and only if $G$ is connected.

**Theorem 5.1.** *Let $G$ and $H$ be two non-trivial connected graphs, then*

$$W_p(G \circ H) = W_p(G)(n(H))^2.$$

*Proof.* Let $u, v \in V(G)$, $x, y \in V(H)$ and $a = (u, x), b = (v, y) \in V(G \circ H)$. Since $G$ is a non-trivial connected graph, then by Lemma 5.1, $G \circ H$ is connected. Note that the lexicographic product $G \circ H$ can be obtained from $G$ by substituting a copy $H_v$ of $H$ for each vertex $v$ of $G$ and by joining all vertices of $H_v$ with all vertices of $H_u$ if $uv \in E(G)$. Therefore, $d_{G \circ H}(a, b) = 3$ if and only if $d_G(u, v) = 3$ and there is a path connecting $x$ and $y$ in $H$. Since $H$ is connected, then

$$W_p(G \circ H) = \frac{2 \times W_p(G)(n(H))^2}{2} = W_p(G)(n(H))^2.$$

The proof is complete. □

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